Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-3-(4-Hexyloxyphenyl)-1-(3-hydroxyphenyl)prop-2-en-one

Zainab Ngaini,[a] Siti Muhaini Haris Fadzillah,[a] Norashikin Irdawaty Abd Rahman,[a] Hasnain Hussain,[b] Ibrahim Abdul Razak[c] and Hoong-Kun Fun[c]*‡

[a]Department of Chemistry, Faculty of Resource Science and Technology, Universiti Malaysia Sarawak, 94300 Kota Samarahan, Sarawak, Malaysia, [b]Department of Molecular Biology, Faculty of Resource Science and Technology, Universiti Malaysia Sarawak, 94300 Kota Samarahan, Sarawak, Malaysia, and [c]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: arazaki@usm.my

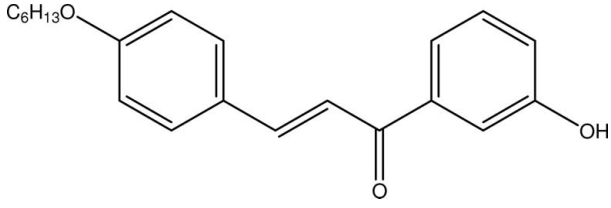
Received 6 March 2009; accepted 23 March 2009

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.043; wR factor = 0.131; data-to-parameter ratio = 34.1.

In the title compound, $C_{21}H_{24}O_3$, the enone unit is in the *s–cis* configuration. The dihedral angle between the benzene rings is 2.18 (4)°. In the crystal, molecules are linked by pairs of O—H···O intermolecular hydrogen bonds, forming inversion dimers. The crystal structure is also consolidated by C—H···π interactions.

Related literature

For general background to the biological properties of chalcone derivatives, see: Bhat *et al.* (2005); Xue *et al.* (2004); Won *et al.* (2005); Yayli *et al.* (2006). For related structures, see: Ng, Razak *et al.* (2006); Ng, Patil *et al.* (2006). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller uded in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{21}H_{24}O_3$
M_r = 324.40
Monoclinic, $P2_1/n$
a = 8.5918 (2) Å
b = 17.1320 (3) Å
c = 12.4192 (2) Å
β = 109.083 (1)°
V = 1727.58 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.52 × 0.43 × 0.37 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.959, T_{max} = 0.970
32772 measured reflections
7567 independent reflections
5739 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.131
S = 1.04
7567 reflections
222 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H101···O2^{i}	0.86 (2)	1.89 (2)	2.739 (1)	171 (2)
C16—H16A···$Cg1^{ii}$	0.97	2.72	3.572 (1)	146
C20—H20A···$Cg1^{iii}$	0.97	2.82	3.642 (1)	143

Symmetry codes: (i) $-x-1, -y, -z$; (ii) $-x, -y, -z+1$; (iii) $-x+1, -y, -z+1$. $Cg1$ is the centroid of C1–C6 ring.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

HKF and IAR thank the Malaysian Government and Universiti Sains Malaysia for the Science Fund grant No. 305/PFIZIK/613312 and the Research University Golden Goose grant No. 1001/PFIZIK/811012. ZN and HH thank Universiti Malaysia Sarawak for the Geran Penyelidikan Dana Khas Inovasi, grant No. DI/01/2007(01). SMHF and NIAR thank the Malaysian Government and Universiti Malaysia Sarawak for providing scholarships for their postgraduate studies.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2200).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* 34, 1555–1573.
Bhat, B. A., Dhar, K. L., Puri, S. C., Saxena, A. K., Shanmugavel, M. & Qazi, G. N. (2005). *Bioorg. Med. Chem. Lett.* **15**, 3177–3180.
Bruker (2005). *APEX2*, *SAINT* and *SADABS* Bruker AXS Inc., Madison, Wisconsin, USA.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Ng, S.-L., Patil, P. S., Razak, I. A., Fun, H.-K. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o1228–o1230.
Ng, S.-L., Razak, I. A., Fun, H.-K., Shettigar, V., Patil, P. S. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o2175–o2177.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

‡ Additional correspondence author, e-mail: hkfun@usm.my.